On mixture approximations for differential equations with distributed time delays

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Outline

1. What are mixture approximations?
   - Three different types of mixture approximations
   - Convergence
   - Practical implementation
   - What can you do with them?
2. Mixture approximations for delay differential equations (DDEs)
   - Examples of DDEs with distributed time delays
   - The linear chain trick (DDEs $\rightarrow$ ODEs)
   - Convergence
   - Simulation example (bifurcation analysis)
   - Kernel identification

Mixture approximations

Problem statement

$\boxed{\text{Approximate the } L^1(\mathcal{D}) \text{ function } \alpha \text{ with the following properties}}$

1. Non-negative and bounded

$$0 \leq \alpha(t) \leq K, \qquad\qquad t \in \mathcal{D}$$

2. Integrates to one

$$\int_{\mathcal{D}} \alpha(t)\,\mathrm{d}t = 1$$

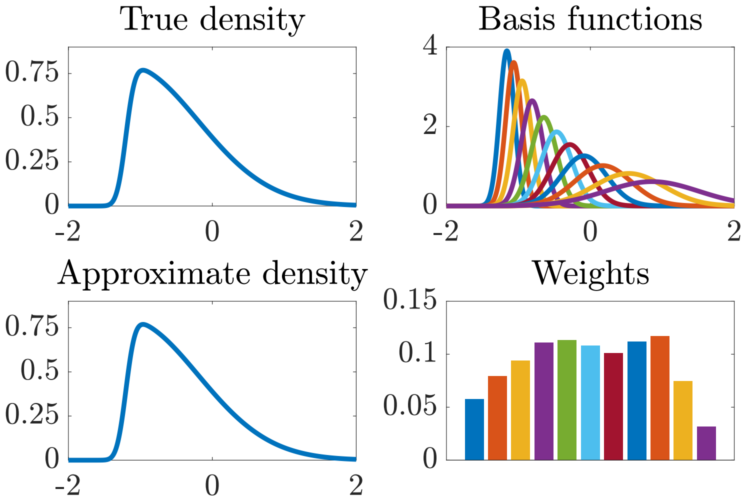
3. Continuous

The domain may be

- the real numbers, $\mathcal{D} = (-\infty, \infty)$,
- the non-negative real numbers, $\mathcal{D} = [0, \infty)$, or
- an interval, $\mathcal{D} = [a, b]$

Example for $\mathcal{D} = (-\infty, \infty)$

Skew normal distribution



Mixture approximation

Approximate α by a sum of basis functions

$$\alpha(t) \approx \hat{\alpha}(t) = \sum_{m=0}^{M} c_m \ell_m(t)$$

Weight constraints

$$\sum_{m=0}^{M} c_m = 1, \qquad 0 \leq c_m \leq 1, \qquad m = 0, \ldots, M$$

Non-negative basis functions

$$\ell_m(t) \geq 0, \qquad m = 0, \ldots, M$$

Basis functions integrate to one

$$\int_{\mathcal{D}} \ell_m(t) \, \mathrm{d}t = 1, \qquad m = 0, \ldots, M$$

Gaussian, Erlang, and beta mixture approximations

Gaussian basis functions, $t \in \mathcal{D} = (-\infty, \infty)$

$$\ell_m(t) = b_m \exp\left(-\frac{1}{2}\left(\frac{t-\mu_m}{\sigma_m}\right)^2\right), \qquad b_m = \frac{1}{\sqrt{2\pi\sigma_m^2}}$$

Erlang basis functions, $t \in \mathcal{D} = [0, \infty)$

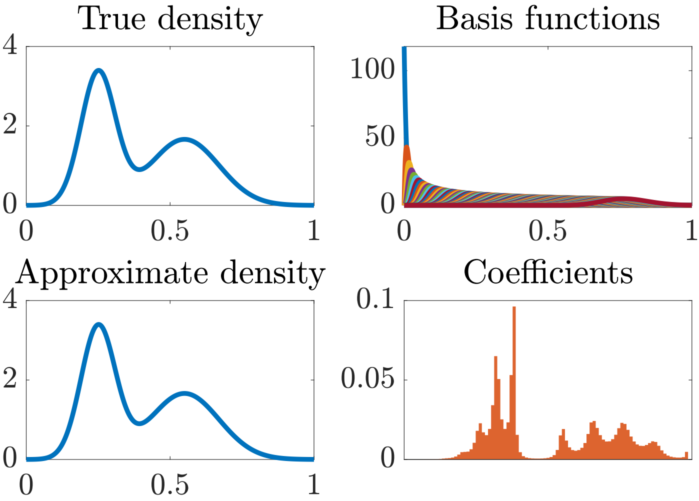
$$\ell_m(t) = b_m t^m e^{-at}, \qquad b_m = \frac{a^{m+1}}{m!}$$

Beta basis functions, $t \in \mathcal{D} = [0, \Delta t]$

$$\ell_m(t) = b_m t^m (\Delta t - t)^{M-m}, \qquad b_m = \frac{1}{\Delta t^{M+1}} \frac{(M+1)!}{m!(M-m)!}$$

Example: Erlang mixture approximation ($M = 90$)

Folded normal mixture distribution



Convergence of Erlang mixture approximations ($M = \infty$)

Coefficients

$$c_m = \int_{s_m}^{s_{m+1}} \alpha(s)\,\mathrm{d}s, \qquad s_m = m\Delta s, \qquad \Delta s = 1/a \tag{1}$$

Weak convergence (Tijms [1, 2])

$$\int_0^t \hat{\alpha}(s)\,\mathrm{d}s \to \int_0^t \alpha(s)\,\mathrm{d}s \quad \text{as} \quad a \to \infty$$

Pointwise convergence (based on delta families [3])

$$\hat{\alpha}(t) \to \alpha(t) \quad \text{as} \quad a \to \infty$$

Vitali's convergence lemma

$$\int_0^\infty |\hat{\alpha}(s) - \alpha(s)|\,\mathrm{d}s \to 0 \quad \text{as} \quad a \to \infty$$

if

- $\hat{\alpha}$ converges pointwise $\checkmark$
- $\hat{\alpha}$ is tight $\checkmark$
- $\hat{\alpha}$ is uniformly integrable $\checkmark$

Convergence of beta and Gaussian mixture approximations

1. Beta mixture approximations, $\mathcal{D} = [0, 1]$
   - ℓ_m is a Bernstein polynomial scaled by $M + 1$
   - pointwise convergence is guaranteed by Weierstrass' approximation theorem [4] as $M \to \infty$

$$c_m = \frac{1}{M+1}\alpha(s_m), \qquad s_m = m\Delta s, \qquad \Delta s = 1/M,$$
$$c_m = \int_{s_m}^{s_{m+1}} \alpha(s)\,\mathrm{d}s, \qquad s_m = m\Delta s, \qquad \Delta s = 1/(M+1)$$

2. Gaussian mixture approximations, $\mathcal{D} = (-\infty, \infty)$
   - Error analysis by Maz'ya and Schmidt [5]
   - Convergence proof by Sorenson and Alspach [6]

Optimal coefficients and rate parameter

Time domain ($k = 0, \ldots, N-1$)

$$\int_0^{t_h} \alpha(s)\,\mathrm{d}s = 1 - \epsilon, \qquad\qquad t_k = k/t_h$$

Least-squares optimization problem

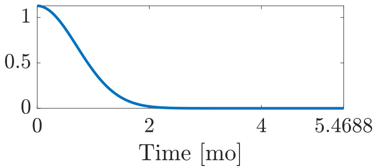
$$\begin{aligned} \min_{\{c_m\}_{m=0}^{M},a} \quad & \phi = \frac{1}{2}\sum_{k=0}^{N-1} (\alpha(t_k) - \hat{\alpha}(t_k))^2 \Delta t, \\ \text{subject to} \quad & \sum_{m=0}^{M} c_m = 1, \\ & 0 \leq c_m \leq 1, \quad m = 0, \ldots, M, \\ & a_{\min} \leq a \end{aligned}$$

- Use Matlab's `fmincon`
- Provide analytical first- and second-order derivatives

Example: Gaussian kernel

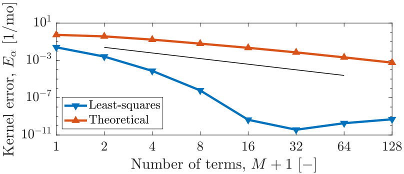
Kernel

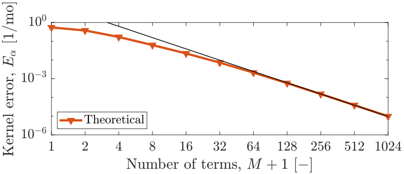
$$\alpha(t) = \frac{2}{\sqrt{\pi}} e^{-t^2}$$



Error

$$E_\alpha = \sum_{k=0}^{N_\alpha - 1} (\hat{\alpha}(t_k) - \alpha(t_k))^2 \Delta t$$





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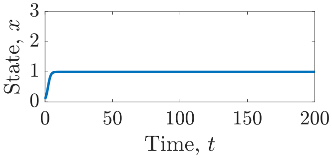
Differential equations with distributed time delays

Delay differential equations

Logistic equation

$$\dot{x}(t) = x(t)\,(1 - x(t))$$

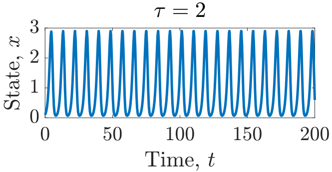


General form (ODE)

$$\dot{x}(t) = f(x(t))$$

Logistic equation w. absolute time delay

$$\dot{x}(t) = x(t)\,(1 - x(t-\tau))$$

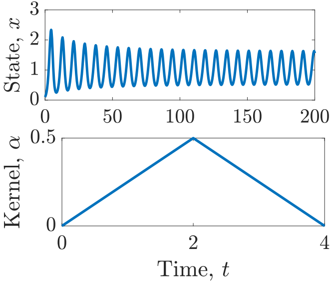


General form (DDE)

$$\dot{x}(t) = f(x(t), x(t-\tau))$$

Logistic equation w. distributed time delay

$$\dot{x}(t) = x(t)\left(1 - \int_{-\infty}^{t} \alpha(t-s)x(s)\,\mathrm{d}s\right)$$



General form (DDDE)

$$\dot{x}(t) = f(x(t), \int_{-\infty}^{t} \alpha(t-s)x(s)\,\mathrm{d}s)$$

Epidemiology

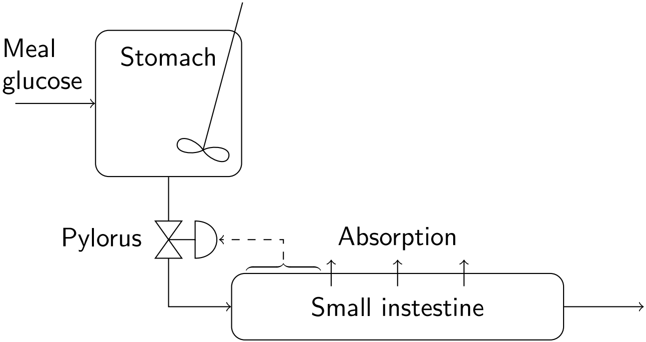
SIR model without delays

$$\begin{aligned}\dot{S}(t) &= -\beta S(t) I(t),\\ \dot{I}(t) &= \beta S(t) I(t) - \eta I(t),\\ \dot{R}(t) &= \eta I(t)\end{aligned}$$

SIR model with distributed time delay

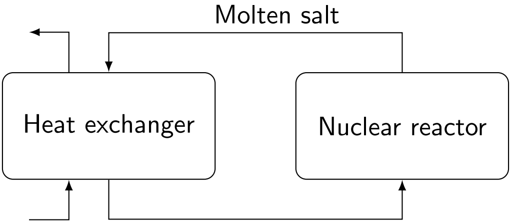
$$\begin{aligned}\dot{S}(t) &= -\beta S(t) \int_{-\infty}^{t} \alpha(t-s) I(s)\,\mathrm{d}s,\\ \dot{I}(t) &= \beta S(t) \int_{-\infty}^{t} \alpha(t-s) I(s)\,\mathrm{d}s - \eta I(t),\\ \dot{R}(t) &= \eta I(t)\end{aligned}$$

Diabetes

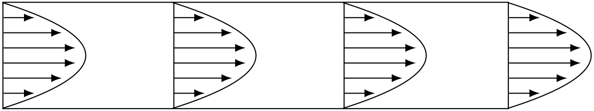


Ritschel, T.K.S., Reenberg, A.T., Carstensen, P.E., Bendsen, J., Jørgensen, J.B., 2023. Mathematical Meal Models for Simulation of Human Metabolism. arXiv: 2307.16444.

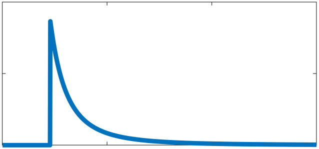
Molten salt nuclear reactor and nonuniform flow in pipes



Non-uniform velocity profile



Kernel for Hagen-Poiseuille flow (quadratic velocity profile)

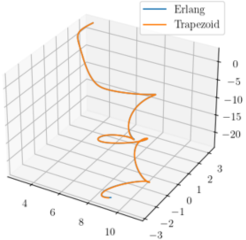


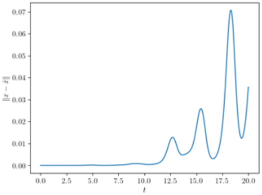
Ritschel, T.K.S., 2025. Numerical Optimal Control for Distributed Delay Differential Equations: A Simultaneous Approach based on Linearization of the Delayed Variables. In: Proceedings of the 2025 European Control Conference (ECC), June 24-27, Thessaloniki, Greece. arXiv: 2410.15083.

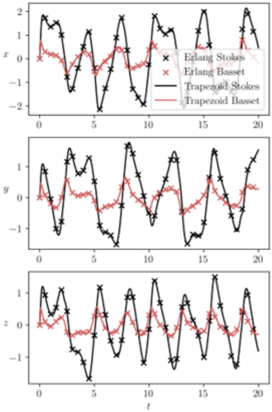
Particle flow in velocity field

Particle subject to Stoke's drag force and Basset history force

$$\dot{x}_p = u_p,$$
$$\dot{u}_p = \underbrace{\frac{1}{\mathrm{St}}\mathcal{F}(a)(u_p - u_f)}_{\text{Nonlinear drag}} + \underbrace{C\int_0^t \frac{1}{\sqrt{t-s}}(\dot{u}_p - \dot{u}_f)\,\mathrm{d}s}_{\text{Basset history force}}$$







Collaboration with PhD candidate Zejian You, Asst. Prof. Qi Wang, and Prof. Gustaaf Jacobs from San Diego State University.

Linear chain trick (DDE $\rightarrow$ ODE)

Linear chain trick

DDE with distributed time delay

$$\dot{x}(t) = f(x(t), z(t)), \qquad z(t) = \int_{-\infty}^{t} \alpha(t-s)x(s)\,\mathrm{d}s$$

Approximate kernel

$$\alpha(t) \approx \hat{\alpha}(t) = \sum_{m=0}^{M} c_m \ell_m(t)$$

Substitute into integral

$$z(t) \approx \hat{z}(t) = \sum_{m=0}^{M} c_m \int_{-\infty}^{t} \ell_m(t-s)x(s)\,\mathrm{d}s = \sum_{m=0}^{M} c_m z_m(t)$$

Differentiate z_m ($\dot{\ell}_0 = -a\ell_0(t)$, $\dot{\ell}_m(t) = a(\ell_{m-1}(t) - \ell_m(t))$)

$$\begin{aligned}\dot{z}_m(t) &= \ell_m(0)x(t) + \int_{-\infty}^{t} \dot{\ell}_m(t-s)x(s)\,\mathrm{d}s \\ &= \begin{cases} a(x(t) - z_0(t)), & m = 0, \\ a(z_{m-1}(t) - z_m(t)), & m > 0 \end{cases}\end{aligned}$$

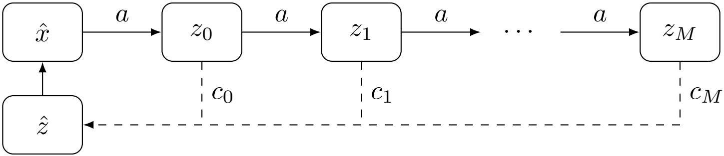
Approximate ODEs

System

$$\dot{\hat{x}}(t) = f(\hat{x}(t), \hat{z}(t)), \qquad \hat{z}(t) = \sum_{m=0}^{M} c_m z_m(t)$$

Auxiliary memory states

$$\begin{aligned} \dot{z}_0(t) &= a(\hat{x}(t) - z_0(t)), \\ \dot{z}_m(t) &= a(z_{m-1}(t) - z_m(t)), \qquad m = 1, \dots, M \end{aligned}$$



Approximate ODEs

Approximate ODEs

$$\begin{aligned}\dot{\hat{x}}(t) &= f(\hat{x}(t), \hat{z}(t)),\\ \dot{Z}(t) &= AZ(t) + B\hat{x}(t),\\ \hat{z}(t) &= CZ(t)\end{aligned}$$

Matrices

$$A = a\begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}, \qquad B = a\begin{bmatrix} 1 \\ \\ \\ \\ \end{bmatrix},$$

$$C = \begin{bmatrix} c_0 & c_1 & \cdots & c_M \end{bmatrix}$$

Does the approximate state converge ($M = \infty$)?

Bound on state error [8, Thm. 1] when f is Lipschitz and x is bounded

$$\int_0^\infty |\hat{\alpha}(t) - \alpha(t)| \, \mathrm{d}t < \epsilon \quad \Rightarrow \quad |\hat{x}(t) - x(t)| \leq \epsilon w(t) \leq \epsilon w(t_f)$$

Auxiliary function

$$\begin{aligned} w(t) &= 0, & t &\in (-\infty, t_0], \\ \dot{w}(t) &= L_z K_x + L_x w(t) + L_z \int_{-\infty}^{t} \hat{\alpha}(t-s) w(s) \, \mathrm{d}s, & t &\in [t_0, t_f] \end{aligned}$$

- The steady state of the approximate ODEs and the DDEs is the same
- The eigenvalues converge to the roots for the DDEs (Hurwitz' convergence theorem)
- Error dynamics are locally stable if the DDEs and ODEs are locally stable

Ritschel, T.K.S., 2025. On Erlang Mixture Approximations for Differential Equations with Distributed Time Delays. arXiv: 2502.12984. In submission.

Numerical example: Simulation

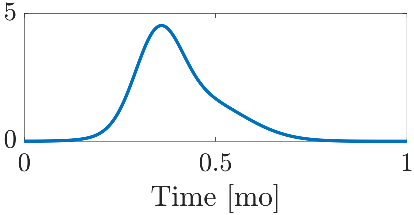
Numerical example

- System

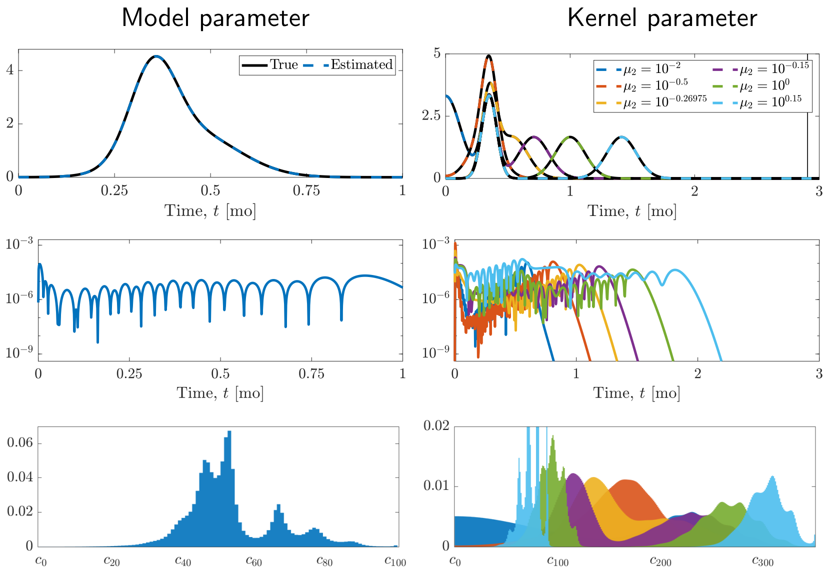
$$\dot{N}(t) = \kappa N(t)\left(1 - \frac{1}{K}\int_{-\infty}^{t} \alpha(t-s)N(s)\,\mathrm{d}s\right)$$

- Kernel

$$\alpha(t) = \gamma_1 F(t;\mu_1,\sigma_1) + \gamma_2 F(t;\mu_2,\sigma_2),$$
$$F(t;\mu,\sigma) = \frac{\exp\left(-\frac{1}{2}\left(\frac{t-\mu}{\sigma}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{t+\mu}{\sigma}\right)^2\right)}{\sqrt{2\pi}\sigma}$$

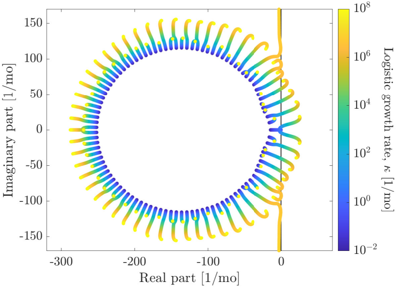


Numerical example: Bifurcation analysis

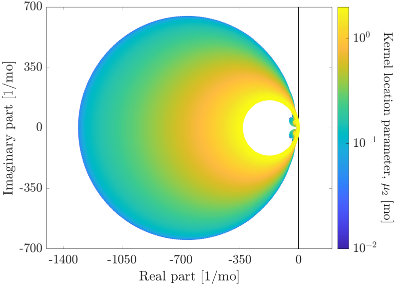


Numerical example: Bifurcation analysis

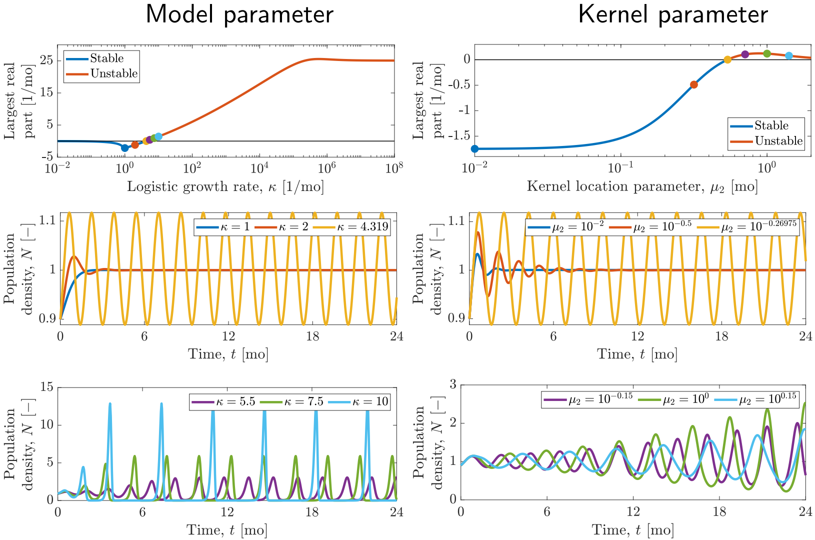
Model parameter



Kernel parameter



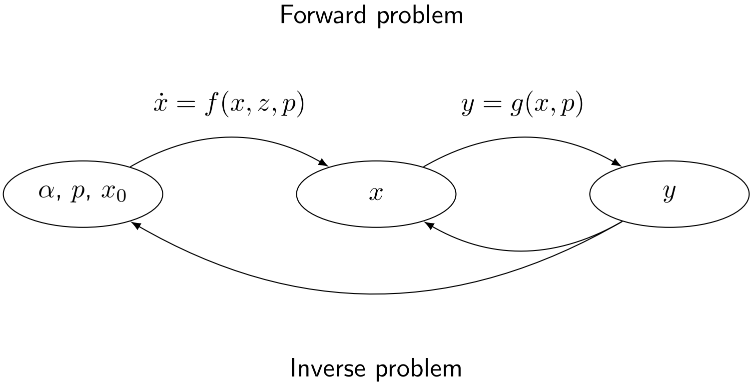
Numerical example: Bifurcation analysis



The numerical simulations are obtained with Euler's implicit method and a right rectangle rule for approximating the integral.

Kernel identification

Kernel identification (with John Wyller, NMBU, Norway)



Ritschel, T.K.S., Wyller, J., 2025. An Algorithm for Distributed Time Delay Identification without A Priori Knowledge of the Kernel. Automatica 178, pp. 112382. DOI: 10.1016/j.automatica.2025.112382.

Dynamical least-squares problem

$$\min_{\{c_m\}_{m=0}^{M}, a, p, x_0} \quad \frac{1}{2} \sum_{k=0}^{N} \|y_k - y(t_k)\|_2^2$$

subject to

$$\begin{aligned}
x(t_0) &= x_0, & & \\
Z(t_0) &= Z_0(x_0, p), & & \\
\dot{x}(t) &= f(x(t), z(t), p), & & t \in [t_0, t_f], \\
\dot{Z}(t) &= AZ(t) + Bx(t), & & t \in [t_0, t_f], \\
z(t) &= CZ(t), & & t \in [t_0, t_f], \\
y(t_k) &= g(x(t_k), p), & & k = 0, \dots, N, \\
\sum_{m=0}^{M} c_m &= 1, & & \\
a_{\min} &\leq a, & & \\
p_{\min} &\leq p \leq p_{\max}, & & \\
x_{\min} &\leq x_0 \leq x_{\max} & &
\end{aligned}$$

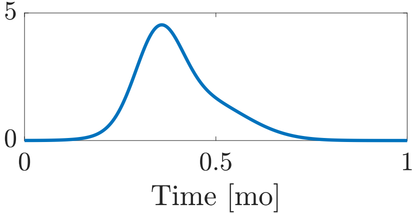
Example

- System

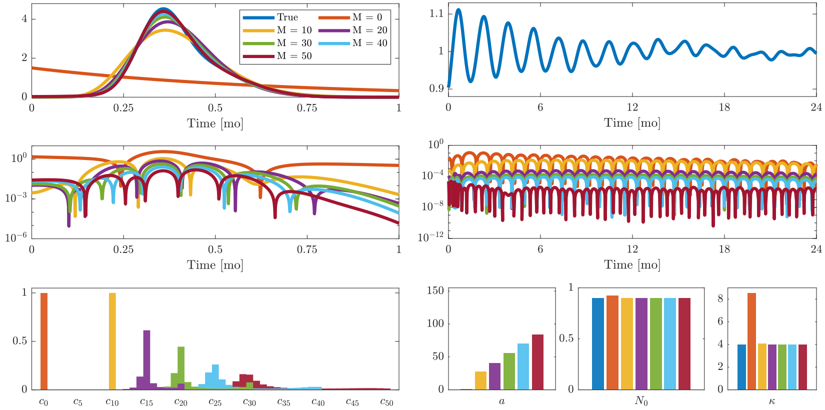
$$\dot{N}(t) = \kappa N(t)\left(1 - \frac{1}{K(t)}\int_{-\infty}^{t} \alpha(t-s)N(s)\,\mathrm{d}s\right),$$
$$K(t) = (1 + A_1\sin(2\pi\omega_1 t) + A_2\sin(2\pi\omega_2 t))\bar{K}$$

- Kernel

$$\alpha(t) = \gamma_1 F(t;\mu_1,\sigma_1) + \gamma_2 F(t;\mu_2,\sigma_2),$$
$$F(t;\mu,\sigma) = \frac{\exp\left(-\frac{1}{2}\left(\frac{t-\mu}{\sigma}\right)^2\right) + \exp\left(-\frac{1}{2}\left(\frac{t+\mu}{\sigma}\right)^2\right)}{\sqrt{2\pi}\sigma}$$



Example



Summary

1. Approximate $L^1(\mathcal{D})$ functions

$$\alpha(t) \approx \hat{\alpha}(t) = \sum_{m=0}^{M} c_m \ell_m(t), \qquad t \in \mathcal{D}$$

2. Approximate solution to DDEs with distributed time delays

$$\dot{x}(t) = f(x(t), \int_{-\infty}^{t} \alpha(t-s) x(s) \, \mathrm{d}s)$$

3. Many different applications/possible extensions
   - Model reduction
   - Stochastic differential equations
   - Continuous thermodynamics (chemical phase/reaction equilibria)
   - Optimal/feedback/adaptive control for DDEs
   - Controllers with memory for ODEs (PID, LQR, MPC, etc.)

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